4-Aminoacridine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.39

Global applicability domain: Inside

Local applicability domain index: 5.18e-01

Confidence level: 6.48e-01

Nearest Neighbors from the Training Set

Image not found
1-Naphthalenol, 2-nitroso-
Measured: 2.46
Predicted: 2.65